8/9/2025

Day 17: The Schrödinger Equation

Let us define an operator $\hat{\tau}(dx')$ such that: $\langle x'+dx'| = \langle x'|\hat{\tau}(dx')$ — (1)

This is called the infinitesimal translation operator. (38) $\Rightarrow$ $|x'+dx'\rangle = \hat{\tau}^{\dagger}(dx')|x'\rangle$ — (2)

Since all the position kets are normalized,

$$\langle x'+dx|x'+dx'\rangle = \langle x'|x'\rangle \quad -(3)$$

$$\Rightarrow \langle x'|\hat{\tau}\hat{\tau}^{\dagger}|x'\rangle = \langle x'|x'\rangle \quad -(4)$$

Since $|x'\rangle$ is arbitrary, (39) implies

$$\hat{\tau}^{\dagger}\hat{\tau} = \hat{1} = \hat{\tau}^{\dagger}\hat{\tau} \quad -(5)$$

Such a matrix is called a unitary matrix.

Now consider an arbitrary state $|\Psi\rangle$

$$\Psi(x') = \langle x'|\Psi\rangle \quad -(6)$$

$$\Psi(x'+dx') = \langle x'+dx'|\Psi\rangle \quad -(7)$$

Since dx' is infinitesimally small we can use Taylor's expansion for (7).

$$\Psi(x'+dx') = \Psi(x') + \frac{d\Psi}{dx'}dx' + O(dx^2) \quad -(8)$$

Using (37) & (42) in (43) we have:

$$\langle x'+dx' | \Psi \rangle = \langle x' | \hat{\tau}(dx') | \Psi \rangle$$

$$= \langle x' | \Psi \rangle + dx' \langle x' | \Phi \rangle + O(dx'^2) \quad -(9)$$

where $|\Phi\rangle$ is the state whose wavefunction is $\frac{d\Psi}{dx'}$ i.e. $\langle x' | \Phi \rangle = \frac{d\Psi}{dx'}$ —(10)

Note that, since

$$\Psi(x') \longrightarrow \frac{d\Psi}{dx'}$$

is a linear map and since these two represent the states $|\Psi\rangle$ & $|\Phi\rangle$, respectively, we can define a linear operator $\hat{D}$:

$$\left.\begin{aligned} &\hat{D}|\Psi\rangle = |\Phi\rangle \\ &\Rightarrow \langle x' | \hat{D} | \Psi \rangle = \Phi(x') = \frac{d\Psi}{dx'} \end{aligned}\right\} -(11)$$

$\therefore$ (9) $\Rightarrow$

$$\langle x' | \hat{\tau}(dx) | \Psi \rangle = \langle x' | \left(\hat{\mathbb{1}} + dx' \hat{D} \right) | \Psi \rangle + O(dx'^2) \quad -(12)$$

Since (12) holds for any state we have the operator identity:

$$\hat{\tau}(dx') \equiv \hat{\mathbb{1}} + dx'\hat{D} \quad — (13)$$

$$\Rightarrow \hat{\tau}^{\dagger}(dx') \equiv \hat{\mathbb{1}} + dx'\hat{D}^{\dagger} \quad — (14)$$

(upto 1st order in dx')

Since $\hat{\tau}$ is unitary,

$$\hat{\mathbb{1}} = \hat{\tau}\hat{\tau}^{\dagger} = (\hat{\mathbb{1}} + dx'\hat{D})(\mathbb{1} + dx'\hat{D}^{\dagger})$$

$$\cong \hat{\mathbb{1}} + dx'(\hat{D} + \hat{D}^{\dagger}) + O(dx'^2) \quad — (15)$$

$$\Rightarrow \hat{D} + \hat{D}' = 0 \text{ or } \boxed{\hat{D} = -\hat{D}^{\dagger}} \quad — (16)$$

i.e. $\hat{D}$ is anti-hermitian

$$\Rightarrow \boxed{\hat{\tau}^{\dagger}(dx') = \hat{\mathbb{1}} - dx'\hat{D}} \quad — (17)$$

(13) $\Rightarrow$

$$[\hat{x}, \hat{\tau}] = dx'[\hat{x}, \hat{D}] \quad — (18)$$

Let's consider the action the operator in (18) on an arbitrary state $|\Psi\rangle$ in $|x\rangle$ basis.

$$\text{LHS} = \langle x' | [\hat{x}, \hat{\mathcal{C}}] | \Psi \rangle$$

$$= x' \langle x' | \hat{\mathcal{C}} | \Psi \rangle - \langle x' | \hat{\mathcal{C}} \hat{x} | \Psi \rangle$$

$$= x' \Psi(x' + dx') - (x' + dx') \Psi(x' + dx')$$

$$= -dx' \Psi(x' + dx')$$

$$= -dx' \left(\Psi(x') + dx' \frac{d\Psi}{dx'} + \cdots \right)$$

$$\simeq -dx' \Psi(x') + O(dx'^2)$$

$$\simeq dx' \langle x' | -\hat{1} | \Psi \rangle \quad \text{— (19)}$$

$$\text{RHS} = \langle x' | [\hat{x}, \hat{D}] | \Psi \rangle \quad \text{— (20)}$$

Comparing the 2 sides we get :

$$\boxed{[\hat{x}, \hat{D}] = -\hat{1}} \quad \text{— (21)}$$

Multiplying both sides by $-i\hbar$ we get

$$\boxed{[\hat{x}, (-i\hbar \hat{D})] = i\hbar} \quad \text{— (22)}$$

Comparing this to our postulate 5,

we get the definition for $\hat{p}_x$

$$\boxed{\hat{p}_x = \frac{\hbar}{i}\hat{p}} \quad \text{— (23)}$$

So that $\boxed{\langle x' | \hat{p}_x | \Psi \rangle = \frac{\hbar}{i}\frac{d\Psi}{dx'}}$ — (24)

Matrix elements of $\hat{p}_x$:

$$\langle x' | \hat{p}_x | \Psi \rangle$$

$$= \int dx'' \overbrace{\langle x' | \hat{p}_x | x'' \rangle}^{P(x', x'')} \Psi(x'')$$

$$= \frac{\hbar}{i}\frac{d\Psi}{dx'} \quad \text{— (25)} \Rightarrow \boxed{\hat{p}_x \leftrightarrow \frac{\hbar}{i}\frac{d}{dx}}$$

$P(x', x'')$ is a function of x'' that yields the derivative of Ψ at x' when integrated over x''. We can determine this function as below.

$$\frac{d\Psi}{dx'} = \int dx'' \, \delta(x'' - x') \, \Psi'(x'')$$

$$\hookrightarrow \frac{d\Psi}{dx''}$$

$$= \left[\delta(x''-x')\,\Psi(x'') \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dx''\, \delta'(x''-x')\,\Psi(x'') \right]$$

(integrating by parts)

$$\text{— } (26)$$

The first term is zero since the Dirac delta function is localized and the wavefunction is usually bound

$$\left(\lim_{x''\to\infty} \Psi(x') = 0 \right)$$

$$\therefore \quad \frac{d\Psi}{dx'} = -\int_{-\infty}^{\infty} dx''\, \delta'(x''-x')\,\Psi(x'') \quad \text{— } (27)$$

Comparing (25) and (27) we get

$$P(x';x'') = \langle x' | \hat{p}_x | x'' \rangle$$

$$= i\hbar\, \delta'(x''-x') \quad \text{— } (28)$$

$\hat{p}_x^2$: $\langle x' | \hat{p}_x^2 | \Psi \rangle$

$$= \int dx'' \langle x' | \hat{p}_x | x'' \rangle \langle x'' | \hat{p}_x | \Psi \rangle$$

$$= i\hbar \int dx'' \, \delta'(x''-x') \, (-i\hbar) \, \Psi'(x'')$$

$$= \hbar^2 \int dx'' \, \delta'(x''-x') \, \Psi'(x'')$$

$$= \hbar^2 \left[\delta(x''-x') \Psi'(x'') \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} dx'' \, \delta(x''-x') \, \Psi''(x'') \right]$$

$$= -\hbar^2 \Psi''(x') = -\hbar^2 \frac{d^2}{dx'^2} \Psi(x') \quad \text{— (29)}$$

$$\Rightarrow \boxed{\hat{p}_x^2 \longleftrightarrow -\hbar^2 \frac{d^2}{dx^2}} \quad \text{— (30)}$$

$$\Rightarrow \hat{T} = \frac{\hat{p}_x^2}{2m} \longrightarrow \frac{-\hbar^2}{2m} \frac{d^2}{dx^2} \quad \text{— (31)}$$

Now, $\hat{p}_x |p_x'\rangle = p_x' |p_x'\rangle$ — (32)

$$\langle x' | \hat{p}_x | p_x' \rangle = p_x' \langle x' | p_x' \rangle$$

$$\Rightarrow -i\hbar \frac{d}{dx'} \psi_{p_x}(x') = p_x' \psi_{p_x}(x') \quad \text{— (33)}$$

where $\psi_{p_x}(x') = \langle x' | p_x' \rangle$ — (34)

is the wavefunction corresponding to the momentum eigenstates.

(60) is a 1^{st} order Differential Equation. Solution is:

$$\psi_{p_x'}(x') = C \exp\left(\frac{i p_x' x'}{\hbar} \right) \quad \text{— (35)}$$

$$\langle p_x' | p_x'' \rangle = \int_{-\infty}^{\infty} dx' \, \psi^*_{p_x'}(x') \, \psi_{p_x''}(x')$$

$$= |C|^2 \int_{-\infty}^{\infty} dx' \exp\left(\frac{i (p_x'' - p_x') x'}{\hbar} \right)$$

$$= \delta(p_x' - p_x'') \quad \text{— (36)}$$

Now, $\frac{1}{2\pi}\int_{-\infty}^{\infty} dx \; e^{ikx} = \delta(k)$ — (37)

$$\therefore \; |c|^2 \int_{-\infty}^{\infty} dx' \exp\left(i \frac{(p_x'' - p_x')x'}{\hbar}\right)$$

$$= |c|^2 \hbar \int_{-\infty}^{\infty} d\left(\frac{x'}{\hbar}\right) \exp\left(i\,(p_x''-p_x')\left(\frac{x'}{\hbar}\right)\right)$$

$$= |c|^2 \, 2\pi\hbar \; \delta(p_x'' - p_x') \quad \text{— (38)}$$

Comparing with the expected result in (63), we get

$$|c|^2 = 1/2\pi\hbar \quad \text{or} \quad |c| = \frac{1}{\sqrt{2\pi\hbar}}$$

$$\therefore \; \psi_{p_x'}(x') = \langle x' | p_x' \rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \exp\left(i \frac{p_x' x'}{\hbar}\right)$$

— (39)